

1-(4-Hydroxyphenyl)-2-(2-oxido-naphthalen-1-yl)diazen-1-ium methanol hemisolvate

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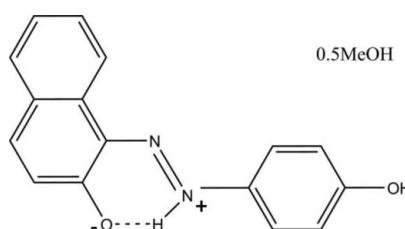
Received 26 April 2013; accepted 5 May 2013

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.002$ Å; disorder in solvent or counterion; R factor = 0.052; wR factor = 0.154; data-to-parameter ratio = 20.9.

In the title compound, $C_{16}H_{12}N_2O_2 \cdot 0.5CH_3OH$, the H atom of the $-OH$ group has been transferred to the N atom in the azo group, forming a zwitterion. Hence, there is an intramolecular $N-H \cdots O$, rather than an $O-H \cdots N$, hydrogen bond in the molecule. The molecule is almost planar, the dihedral angle between the benzene ring and the mean plane of the naphthalene ring system being $4.51(6)^\circ$. In the crystal, molecules are linked to and bridged by $O-H \cdots O$ hydrogen bonds involving the methanol molecule, which is located about a twofold rotation axis, and hence half-occupied, forming zigzag chains along [001]. Molecules are also linked via $C-H \cdots \pi$ and $\pi-\pi$ interactions, the latter involving adjacent benzene and naphthalene rings and having a centroid-centroid distance of $3.6616(13)$ Å, forming a three-dimensional network.

Related literature

For azo compounds in the fields of dyes, pigments and advanced materials, see: Lee *et al.* (2004); Oueslati *et al.* (2004). For the synthesis of azo compounds, see: Wang *et al.* (2003). For the structures of related compounds, see: Jin *et al.* (2008); Xu *et al.* (2010).



Experimental

Crystal data

$C_{16}H_{12}N_2O_2 \cdot 0.5CH_3OH$
 $M_r = 280.30$
Monoclinic, $C2/c$
 $a = 26.942(7)$ Å
 $b = 6.3479(17)$ Å
 $c = 17.579(5)$ Å
 $\beta = 113.985(4)^\circ$

$V = 2746.8(13)$ Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 293$ K
 $0.26 \times 0.06 \times 0.05$ mm

Data collection

Bruker APEXII CCD
diffractometer
12992 measured reflections
4212 independent reflections
2286 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.154$
 $S = 1.03$
4212 reflections
202 parameters
H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³

Table 1
Hydrogen-bond geometry (Å, °).

$Cg2$ and $Cg3$ are the centroids of the C5–C10 and C11–C16 rings, respectively.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1S–H1O \cdots O1 ⁱ	0.92	1.92	2.832 (3)	171
N2–H2A \cdots O1	0.86	1.84	2.540 (2)	137
O2–H2B \cdots O1S	0.82	2.03	2.841 (3)	172
O2–H2B \cdots O1S ⁱⁱ	0.82	1.97	2.690 (3)	146
C1S–H1SA \cdots Cg3 ⁱⁱⁱ	1.11 (6)	2.58 (5)	3.555 (2)	147 (4)
C7–H7A \cdots Cg2 ^{iv}	0.93	2.73	3.521 (2)	144

Symmetry codes: (i) $-x, -y + 3, -z$; (ii) $-x, y, -z - \frac{1}{2}$; (iii) $-x, y + 1, -z - \frac{1}{2}$; (iv) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012).

The authors, particularly MB (PNR project), thank the MESRS (Algeria) for financial support. Thanks are also due to Professor Ouahab, Director of Research at the Laboratory UMR LCSIM 6511, CNRS, Rennes I (France) for recording the diffraction data and help with the structure determination.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2594).

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supplementary materials

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1-(4-Hydroxyphenyl)-2-(2-oxidonaphthalen-1-yl)diazen-1-ium methanol hemisolvate

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Comment

Azo compounds are very important in the fields of dyes, pigments and advanced materials (Lee *et al.*, 2004; Oueslati *et al.*, 2004). Characterized by the azo linkage (–N=N–). Many azo compounds have been synthesized by the diazotization and a diazo coupling reaction (Wang *et al.*, 2003), followed by a coupling reaction with 2-naphthol. This entails an electrophilic substitution reaction where an aryl diazonium cation attacks another aryl ring. Since diazonium salts are often unstable near room temperature, the azo coupling reactions are typically conducted near ice temperatures. The pH of the solution is quite important; it must be mildly acidic or neutral, since no reaction takes place if the pH is too low. We report herein on the crystal structure of the title compound, obtained through the diazotization of 4-hydroxyaniline followed by a coupling reaction with 2-naphthol. The synthesis and structure of a 4-methylaniline (Wang *et al.*, 2003) and an aniline (Jin *et al.*, 2008; Xu *et al.*, 2010) analogue of the title compound have been described.

In the title molecule, Fig. 1, the bond lengths and angles are within normal ranges. Interestingly, the hydrogen atom of the OH group has been transferred to the N2 atom in the azo group to form a dipolar ion; the difference Fourier map indicated that the hydrogen atom site location is closer to the N atom of the azo group. Hence, there is an intramolecular N—H···O, rather than an O—H···N, hydrogen bond in the molecule (Fig. 1 and Table 1). The molecule is relatively plane, with mean plane of the naphthalene ring system (C1–C10) oriented at a dihedral angle of 4.51 (6) ° with respect to the benzene ring (C11–C16).

In the crystal, molecules are bridged by O—H···O hydrogen bonds, involving the methanol molecule which is located about a twofold rotation axis, forming chains along [001]; see Table 1 and Fig. 2. Molecules are also linked via C—H···π (Table 1) and π···π interactions interactions, forming a three-dimensional structure. The latter interactions involve adjacent benzene and naphthalene rings [Cg1···Cg3ⁱ = 3.6616 (13) Å; Cg1 is the centroid of ring C1–C6; Cg3 is the centroid of ring C11–C16; symmetry code: (i) x, y–1, z].

Experimental

The title compound was prepared by the method of (Wang *et al.*, 2003) for similar aromatic azo–compounds. Red prismatic crystals of the title compound were obtained by slow evaporation of a solution in methanol.

Refinement

The hydrogen atom of the OH group was located in a difference Fourier map and found to be near to the N atom, N2, of the azo group. In the final cycles of refinement it was included in a calculated position and treated as a riding atom: N—H = 0.86 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. The C-bound H atoms were positioned geometrically and refined as riding: C—H = 0.93 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The disordered methanol solvent OH and CH₃ H atoms were located in a difference Fourier map and refined as riding atoms with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O,C})$. Two reflections (2 0 0 and 1 1 3) likely affected by

the beamstop were omitted in the final cycles of refinement.

Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012).

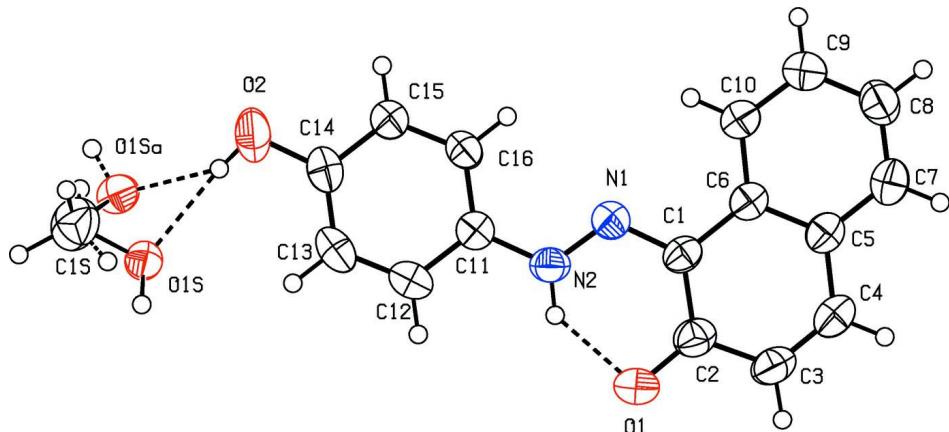
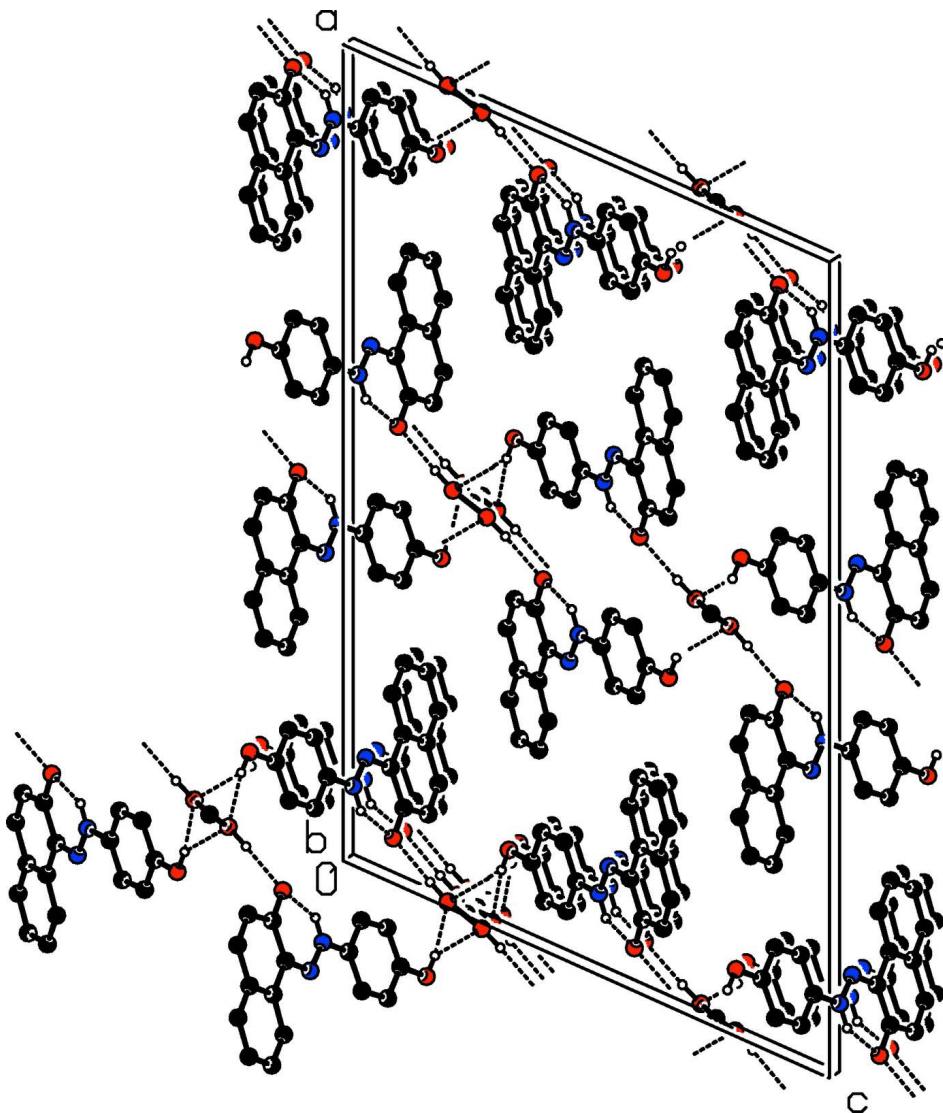


Figure 1

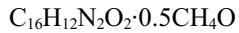
View of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

A view along the axis of the crystal packing of the title compound. The various hydrogen bonds are shown as dashed lines (see Table 1 for details).

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Crystal data



$M_r = 280.30$

Monoclinic, $C2/c$

Hall symbol: -C 2yc

$a = 26.942 (7) \text{ \AA}$

$b = 6.3479 (17) \text{ \AA}$

$c = 17.579 (5) \text{ \AA}$

$\beta = 113.985 (4)^\circ$

$V = 2746.8 (13) \text{ \AA}^3$

$Z = 8$

$F(000) = 1176$

Least-squares treatment of 25 SET4 setting angles.

$D_x = 1.356 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1832 reflections

$\theta = 2.4\text{--}25.7^\circ$

$\mu = 0.09 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Prismatic, red

$0.26 \times 0.06 \times 0.05 \text{ mm}$

Data collection

Bruker APEXII CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
12992 measured reflections
4212 independent reflections

2286 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\text{max}} = 30.7^\circ, \theta_{\text{min}} = 2.4^\circ$
 $h = -38 \rightarrow 37$
 $k = -8 \rightarrow 9$
 $l = -24 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.154$
 $S = 1.03$
4212 reflections
202 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.3604P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.05411 (5)	0.9010 (2)	0.10115 (8)	0.0693 (5)	
O2	0.09325 (5)	1.7942 (2)	-0.17549 (9)	0.0775 (5)	
N1	0.13875 (5)	0.98315 (19)	0.04654 (7)	0.0426 (4)	
N2	0.09869 (5)	1.1128 (2)	0.02339 (7)	0.0454 (4)	
C1	0.13793 (5)	0.8158 (2)	0.09375 (8)	0.0408 (4)	
C2	0.09520 (6)	0.7749 (3)	0.12016 (10)	0.0516 (5)	
C3	0.09810 (7)	0.5873 (3)	0.16635 (10)	0.0563 (6)	
C4	0.13956 (6)	0.4517 (3)	0.18484 (9)	0.0510 (5)	
C5	0.18354 (6)	0.4878 (2)	0.16088 (8)	0.0439 (5)	
C6	0.18351 (5)	0.6722 (2)	0.11622 (8)	0.0402 (4)	
C7	0.22698 (6)	0.3453 (3)	0.18175 (9)	0.0529 (5)	
C8	0.26920 (7)	0.3855 (3)	0.16014 (10)	0.0590 (6)	
C9	0.26971 (6)	0.5681 (3)	0.11681 (10)	0.0565 (6)	
C10	0.22765 (6)	0.7090 (3)	0.09506 (9)	0.0482 (5)	
C11	0.09846 (5)	1.2857 (2)	-0.02644 (8)	0.0421 (4)	
C12	0.05513 (6)	1.4243 (3)	-0.04920 (10)	0.0505 (5)	
C13	0.05257 (6)	1.5962 (3)	-0.09868 (10)	0.0555 (5)	
C14	0.09319 (6)	1.6298 (2)	-0.12578 (9)	0.0507 (5)	

C15	0.13698 (6)	1.4922 (2)	-0.10218 (9)	0.0497 (5)	
C16	0.13961 (6)	1.3214 (2)	-0.05285 (9)	0.0467 (5)	
O1S	-0.00722 (9)	2.0049 (3)	-0.21505 (14)	0.0490 (7)	0.500
C1S	0.00000	2.1846 (5)	-0.25000	0.0803 (14)	
H2A	0.07230	1.09380	0.03830	0.0540*	
H2B	0.06390	1.85490	-0.19190	0.1160*	
H3A	0.07060	0.55830	0.18400	0.0680*	
H4A	0.13970	0.32990	0.21430	0.0610*	
H7A	0.22690	0.22250	0.21060	0.0630*	
H8A	0.29780	0.29040	0.17440	0.0710*	
H9A	0.29880	0.59470	0.10250	0.0680*	
H10A	0.22840	0.83040	0.06590	0.0580*	
H12A	0.02760	1.40130	-0.03110	0.0610*	
H13A	0.02350	1.68920	-0.11370	0.0670*	
H15A	0.16470	1.51600	-0.11990	0.0600*	
H16A	0.16900	1.22980	-0.03720	0.0560*	
H1SA	-0.035 (2)	2.289 (9)	-0.284 (3)	0.1210*	0.500
H1O	-0.02100	2.04990	-0.17790	0.0740*	0.500
H1SB	0.0081 (13)	2.124 (4)	-0.2876 (18)	0.1210*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0529 (7)	0.0772 (9)	0.0909 (9)	0.0092 (6)	0.0428 (6)	0.0195 (7)
O2	0.0765 (9)	0.0569 (8)	0.0916 (9)	0.0183 (7)	0.0265 (8)	0.0293 (7)
N1	0.0401 (6)	0.0436 (7)	0.0416 (6)	-0.0025 (5)	0.0140 (5)	-0.0025 (5)
N2	0.0390 (6)	0.0523 (8)	0.0480 (7)	-0.0009 (6)	0.0209 (5)	0.0012 (6)
C1	0.0407 (7)	0.0440 (8)	0.0368 (7)	-0.0082 (6)	0.0148 (6)	-0.0020 (6)
C2	0.0462 (8)	0.0579 (10)	0.0513 (8)	-0.0068 (7)	0.0206 (7)	0.0019 (8)
C3	0.0542 (9)	0.0640 (11)	0.0575 (9)	-0.0095 (8)	0.0298 (8)	0.0059 (8)
C4	0.0584 (9)	0.0525 (10)	0.0423 (8)	-0.0109 (8)	0.0207 (7)	0.0026 (7)
C5	0.0480 (8)	0.0463 (9)	0.0346 (7)	-0.0061 (7)	0.0139 (6)	-0.0019 (6)
C6	0.0420 (7)	0.0431 (8)	0.0339 (7)	-0.0057 (6)	0.0137 (5)	-0.0033 (6)
C7	0.0627 (10)	0.0472 (9)	0.0451 (8)	-0.0005 (8)	0.0181 (7)	0.0033 (7)
C8	0.0598 (10)	0.0561 (11)	0.0604 (10)	0.0137 (8)	0.0238 (8)	0.0054 (8)
C9	0.0508 (9)	0.0624 (11)	0.0618 (10)	0.0030 (8)	0.0284 (8)	0.0031 (8)
C10	0.0495 (8)	0.0500 (9)	0.0486 (8)	-0.0012 (7)	0.0235 (7)	0.0034 (7)
C11	0.0420 (7)	0.0430 (8)	0.0392 (7)	-0.0017 (6)	0.0144 (6)	-0.0034 (6)
C12	0.0401 (7)	0.0571 (10)	0.0548 (9)	0.0040 (7)	0.0197 (7)	-0.0062 (8)
C13	0.0443 (8)	0.0492 (10)	0.0638 (10)	0.0121 (7)	0.0124 (7)	-0.0031 (8)
C14	0.0518 (9)	0.0412 (9)	0.0516 (8)	0.0063 (7)	0.0134 (7)	0.0015 (7)
C15	0.0509 (8)	0.0481 (9)	0.0544 (9)	0.0072 (7)	0.0259 (7)	0.0060 (7)
C16	0.0436 (7)	0.0472 (9)	0.0506 (8)	0.0105 (7)	0.0205 (6)	0.0050 (7)
O1S	0.0556 (12)	0.0450 (13)	0.0529 (12)	0.0055 (11)	0.0286 (10)	0.0051 (10)
C1S	0.105 (3)	0.058 (2)	0.090 (2)	0.0000	0.052 (2)	0.0000

Geometric parameters (\AA , ^\circ)

O1—C2	1.295 (2)	C11—C16	1.384 (2)
O2—C14	1.362 (2)	C11—C12	1.385 (2)

O2—H2B	0.8200	C12—C13	1.380 (3)
O1S—C1S	1.347 (3)	C13—C14	1.376 (2)
O1S—H1SB ⁱ	0.76 (3)	C14—C15	1.389 (2)
O1S—H1O	0.9200	C15—C16	1.372 (2)
N1—N2	1.2848 (19)	C3—H3A	0.9300
N1—C1	1.3538 (18)	C4—H4A	0.9300
N2—C11	1.4027 (18)	C7—H7A	0.9300
N2—H2A	0.8600	C8—H8A	0.9300
C1—C6	1.449 (2)	C9—H9A	0.9300
C1—C2	1.429 (2)	C10—H10A	0.9300
C2—C3	1.426 (3)	C12—H12A	0.9300
C3—C4	1.341 (3)	C13—H13A	0.9300
C4—C5	1.428 (2)	C15—H15A	0.9300
C5—C7	1.405 (2)	C16—H16A	0.9300
C5—C6	1.4093 (19)	C1S—H1SA	1.11 (6)
C6—C10	1.402 (2)	C1S—H1SB	0.87 (3)
C7—C8	1.362 (3)	C1S—H1SA ⁱ	1.11 (6)
C8—C9	1.390 (3)	C1S—H1SB ⁱ	0.87 (3)
C9—C10	1.370 (3)		
C14—O2—H2B	109.00	C4—C3—H3A	119.00
C1S—O1S—H1O	104.00	C2—C3—H3A	119.00
C1S—O1S—H1SB ⁱ	37 (2)	C3—C4—H4A	119.00
H1O—O1S—H1SB ⁱ	67.00	C5—C4—H4A	119.00
N2—N1—C1	118.42 (14)	C5—C7—H7A	120.00
N1—N2—C11	119.27 (13)	C8—C7—H7A	120.00
N1—N2—H2A	120.00	C9—C8—H8A	120.00
C11—N2—H2A	120.00	C7—C8—H8A	120.00
C2—C1—C6	120.15 (13)	C8—C9—H9A	120.00
N1—C1—C2	123.90 (14)	C10—C9—H9A	120.00
N1—C1—C6	115.94 (13)	C6—C10—H10A	120.00
O1—C2—C1	121.39 (16)	C9—C10—H10A	120.00
O1—C2—C3	120.43 (16)	C11—C12—H12A	120.00
C1—C2—C3	118.16 (16)	C13—C12—H12A	120.00
C2—C3—C4	121.44 (18)	C12—C13—H13A	120.00
C3—C4—C5	122.32 (16)	C14—C13—H13A	120.00
C4—C5—C7	121.51 (14)	C16—C15—H15A	120.00
C6—C5—C7	119.48 (15)	C14—C15—H15A	120.00
C4—C5—C6	119.01 (14)	C11—C16—H16A	120.00
C1—C6—C5	118.87 (13)	C15—C16—H16A	120.00
C1—C6—C10	122.60 (13)	O1S—C1S—O1S ⁱ	64.2 (2)
C5—C6—C10	118.53 (14)	O1S—C1S—H1SA	120 (3)
C5—C7—C8	120.54 (16)	O1S—C1S—H1SB	95.7 (18)
C7—C8—C9	120.30 (18)	O1S—C1S—H1SA ⁱ	121 (3)
C8—C9—C10	120.39 (17)	O1S—C1S—H1SB ⁱ	31.5 (18)
C6—C10—C9	120.76 (16)	H1SA—C1S—H1SB	106 (3)
N2—C11—C12	117.83 (14)	O1S ⁱ —C1S—H1SA	121 (3)
N2—C11—C16	122.48 (13)	H1SA—C1S—H1SA ⁱ	107 (4)
C12—C11—C16	119.70 (13)	H1SA—C1S—H1SB ⁱ	105 (4)

C11—C12—C13	120.33 (16)	O1S ⁱ —C1S—H1SB	31.5 (18)
C12—C13—C14	119.86 (16)	H1SA ⁱ —C1S—H1SB	105 (4)
O2—C14—C13	123.34 (15)	H1SB—C1S—H1SB ⁱ	127 (3)
C13—C14—C15	119.84 (14)	O1S ⁱ —C1S—H1SA ⁱ	120 (3)
O2—C14—C15	116.82 (15)	O1S ⁱ —C1S—H1SB ⁱ	95.7 (18)
C14—C15—C16	120.34 (16)	H1SA ⁱ —C1S—H1SB ⁱ	106 (3)
C11—C16—C15	119.93 (14)		
C1—N1—N2—C11	−179.19 (12)	C7—C5—C6—C1	178.85 (13)
N2—N1—C1—C2	−0.5 (2)	C7—C5—C6—C10	−1.0 (2)
N2—N1—C1—C6	178.51 (12)	C4—C5—C7—C8	−178.29 (15)
N1—N2—C11—C12	−178.98 (13)	C6—C5—C7—C8	0.9 (2)
N1—N2—C11—C16	0.9 (2)	C1—C6—C10—C9	−179.35 (14)
N1—C1—C2—O1	−1.3 (2)	C5—C6—C10—C9	0.5 (2)
N1—C1—C2—C3	177.00 (14)	C5—C7—C8—C9	−0.2 (2)
C6—C1—C2—O1	179.78 (14)	C7—C8—C9—C10	−0.3 (3)
C6—C1—C2—C3	−2.0 (2)	C8—C9—C10—C6	0.2 (2)
N1—C1—C6—C5	−176.08 (12)	N2—C11—C12—C13	−179.50 (14)
N1—C1—C6—C10	3.72 (19)	C16—C11—C12—C13	0.7 (2)
C2—C1—C6—C5	2.97 (19)	N2—C11—C16—C15	179.40 (13)
C2—C1—C6—C10	−177.23 (14)	C12—C11—C16—C15	−0.8 (2)
O1—C2—C3—C4	178.23 (16)	C11—C12—C13—C14	0.2 (2)
C1—C2—C3—C4	0.0 (2)	C12—C13—C14—O2	179.21 (15)
C2—C3—C4—C5	1.1 (3)	C12—C13—C14—C15	−0.9 (2)
C3—C4—C5—C6	0.0 (2)	O2—C14—C15—C16	−179.31 (13)
C3—C4—C5—C7	179.16 (15)	C13—C14—C15—C16	0.8 (2)
C4—C5—C6—C1	−1.97 (19)	C14—C15—C16—C11	0.0 (2)
C4—C5—C6—C10	178.22 (13)		

Symmetry code: (i) $-x, y, -z-1/2$.

Hydrogen-bond geometry (Å, °)

Cg2 and Cg3 are the centroids of the C5—C10 and C11—C16 rings, respectively.

$D\cdots H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O1S—H1O ⁱⁱ —O1 ⁱⁱ	0.92	1.92	2.832 (3)	171
N2—H2A ⁱⁱⁱ —O1	0.86	1.84	2.540 (2)	137
O2—H2B ⁱⁱⁱ —O1S	0.82	2.03	2.841 (3)	172
O2—H2B ⁱⁱⁱ —O1S ⁱ	0.82	1.97	2.690 (3)	146
C1S—H1SA ^{iv} —Cg3 ⁱⁱⁱ	1.11 (6)	2.58 (5)	3.555 (2)	147 (4)
C7—H7A ^{iv} —Cg2 ^{iv}	0.93	2.73	3.521 (2)	144

Symmetry codes: (i) $-x, y, -z-1/2$; (ii) $-x, -y+3, -z$; (iii) $-x, y+1, -z-1/2$; (iv) $-x+1/2, y-1/2, -z+1/2$.